Glutaric acid, 2-(3-bromophenyl)ethyl isobutyl ester

Inchi: InChI=1S/C17H23BrO4/c1-13(2)12-22-17(20)8-4-7-16(19)21-10-9-14-5-3-6-15(18)11-14/

InchiKey: AEELWTYLNKCUJI-UHFFFAOYSA-N

Formula: C17H23BrO4

SMILES: CC(C)COC(=O)CCCC(=O)OCCc1cccc(Br)c1

Mol. weight [g/mol]: 371.27

Physical Properties

Property code	Value	Unit	Source
gf	-260.92	kJ/mol	Joback Method
hf	-637.70	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.904		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	838.32	K	Joback Method
tc	1051.65	K	Joback Method
tf	509.41	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.57	J/mol×K	838.32	Joback Method
cpg	803.77	J/mol×K	1016.09	Joback Method
cpg	793.97	J/mol×K	980.54	Joback Method
cpg	783.18	J/mol×K	944.98	Joback Method
cpg	771.36	J/mol×K	909.43	Joback Method
cpg	758.50	J/mol×K	873.87	Joback Method
cpg	812.60	J/mol×K	1051.65	Joback Method
dvisc	0.0000612	Pa×s	838.32	Joback Method

dvisc	0.0000782	Pa×s	783.50	Joback Method
dvisc	0.0001039	Pa×s	728.68	Joback Method
dvisc	0.0001444	Pa×s	673.87	Joback Method
dvisc	0.0002129	Pa×s	619.05	Joback Method
dvisc	0.0003384	Pa×s	564.23	Joback Method
dvisc	0.0005943	Pa×s	509.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume